

# On the Efficiency of Quantum Algorithms for Hamiltonian Simulation

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We study the efficiency of algorithms simulating a system evolving with Hamiltonian  $H = \sum_{j=1}^m H_j$ . We consider high order splitting methods that play a key role in quantum Hamiltonian simulation. We obtain upper bounds on the number of exponentials required to approximate  $e^{-iHt}$  with error  $\varepsilon$ . Moreover, we derive the order of the splitting method that optimizes the cost of the resulting algorithm. We show significant speedups relative to previously known results.

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## I. INTRODUCTION

While the computational cost of simulating many particle quantum systems using classical computers grows exponentially with the number of particles, quantum computers have the potential to carry out the simulation efficiently [1–4]. This property, pointed out by Feynman, is one of the fundamental ideas of the field of quantum computation. The simulation problem is also related to quantum walks and adiabatic optimization [5–10].

A variety of quantum algorithms have been proposed to predict and simulate the behavior of different physical and chemical systems. Of particular interest are *splitting methods* that simulate the unitary evolution  $e^{-iHt}$ , where  $H$  is the system Hamiltonian, by a product of unitary operators of the form  $e^{-iA_l t_l}$ , for some  $t_l$ ,  $l = 1, \dots, N$ , where  $A_l \in \{H_1, \dots, H_m\}$ ,  $H = \sum_{j=1}^m H_j$  and assuming the Hamiltonians  $H_j$  do not commute. It is further assumed that the  $H_j$  can be implemented efficiently. Throughout this paper we assume that the  $H_j$  are either Hermitian matrices or bounded Hermitian operators so that  $\|H_j\| < \infty$  for  $j = 1, \dots, m$ , where  $\|\cdot\|$  is an induced norm [17].

As Nielsen and Chuang [11, p. 207] point out, the heart of quantum simulation is in the Lie-Trotter formula

$$\lim_{n \rightarrow \infty} (e^{-iH_1 t/n} e^{-iH_2 t/n})^n = e^{-i(H_1+H_2)t}.$$

From this one obtains the second order approximation

$$e^{-i(H_1+H_2)\Delta t} = e^{-iH_1 \Delta t} e^{-iH_2 \Delta t} + O(|\Delta t|^2).$$

A third order approximation is given by the Strang splitting

$$e^{-i(H_1+H_2)\Delta t} = e^{-iH_1 \Delta t/2} e^{-iH_2 \Delta t} e^{-iH_1 \Delta t/2} + O(|\Delta t|^3).$$

Suzuki [12, 13] uses recursive modifications of this approximation to derive methods of order  $2k + 1$ , for  $k = 1, 2, \dots$ .

A recent paper [4] shows that Suzuki's high order splitting methods can be used to derive bounds for the number  $N$  of exponentials, assuming the  $H_j$  are local Hamiltonians. These

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bounds are expressed in terms of the evolution time  $t$ , the norm  $\|H\|$  of the Hamiltonian  $H$ , the order of the splitting method  $2k + 1$ , the number of Hamiltonians  $m$ , and the error  $\varepsilon$  in the approximation of  $e^{-iHt}$ . In this paper we will show how these bounds can be significantly improved.

Consider the Hamiltonians indexed with respect to the magnitude of their norms  $\|H_1\| \geq \|H_2\| \geq \dots \geq \|H_m\|$ . Then the number of necessary exponentials  $N$  generally depends on  $H_1$ , but it must also depend explicitly on  $H_2$  since only one exponential should suffice for the simulation if  $\|H_2\| \rightarrow 0$ . This observation is particularly important for the simulation of systems in physics and chemistry. To see this, suppose  $m = 2$  and that  $H_1$  is a discretization of the negative Laplacian  $-\Delta$ , while  $H_2$  is a discretization of a uniformly bounded potential. Then  $e^{-iH_1t_1}$  and  $e^{-iH_2t_2}$  can be implemented efficiently for any  $t_1, t_2$ , and  $\|H_2\| \ll \|H_1\|$ . We will see that, not only in this case but in general, the number of exponentials is proportional to both  $\|H_1\|$  and  $\|H_2\|$ , i.e., the Hamiltonian of the second largest norm plays an important role.

Let  $\varepsilon$  be sufficiently small. The previously known bound for the number of exponentials, according to [4], is

$$N \leq N_{\text{prev}} := m5^{2k}(m\|H\|t)^{1+\frac{1}{2k}}\varepsilon^{-1/(2k)}. \quad (1)$$

This bound does not properly reflect the dependence on  $H_2$ .

Performing a more detailed analysis of the approximation error by high order splitting formulas, it is possible to improve the bounds for  $N$  substantially. The new estimates lead to *optimal* splitting methods of significantly lower order which greatly reduces the cost of the algorithms.

We now summarize our results. Recall that the  $H_j$  can be implemented efficiently but do not commute and  $\|H_1\| \geq \|H_2\| \geq \dots \geq \|H_m\|$ . We show the following:

1. A new bound for the number of exponentials  $N$ , given by

$$N \leq N_{\text{new}} := 2(2m - 1) 5^{k-1} \|H_1\| t \left( \frac{4emt\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{4me}{3} \left( \frac{5}{3} \right)^{k-1}.$$

2. A speedup factor of

$$\frac{N_{\text{new}}}{N_{\text{prev}}} \leq \frac{2}{3^k} \left( \frac{4e\|H_2\|}{\|H_1\|} \right)^{1/2k}.$$

3. We show that the *optimal*  $k_{\text{new}}^*$  that minimizes  $N_{\text{new}}$  is

$$k_{\text{new}}^* := \text{round} \left( \sqrt{\frac{1}{2} \log_{25/3} \frac{4emt\|H_2\|}{\varepsilon}} \right).$$

On the other hand, from [4] the bound for  $N_{\text{prev}}$  is minimized for

$$k_{\text{prev}}^* = \text{round} \left( \frac{1}{2} \sqrt{\log_5 \frac{m\|H\|t}{\varepsilon} + 1} \right).$$

4. For  $k_{\text{new}}^*$  the value of  $N_{\text{new}}$  satisfies

$$N_{\text{new}}^* \leq \frac{8}{3} (2m - 1) met \|H_1\| e^{2\sqrt{\frac{1}{2} \ln \frac{25}{3} \ln \frac{4emt\|H_2\|}{\varepsilon}}}.$$

For  $k_{\text{prev}}^*$  the value of  $N_{\text{prev}}$  is

$$N_{\text{prev}}^* = 2m^2 \|H\| t \cdot e^{2\sqrt{\ln 5 \ln(m\|H\|t/\epsilon)}}.$$

Hence

$$\frac{N_{\text{new}}^*}{N_{\text{prev}}^*} \leq \frac{8e}{3} e^{2\left(\sqrt{\frac{1}{2} \ln \frac{25}{3} \ln \frac{4emt\|H_2\|}{\epsilon}} - \sqrt{\ln 5 \ln \frac{m\|H_1\|t}{\epsilon}}\right)}.$$

## II. SPLITTING METHODS FOR SIMULATING THE SUM OF TWO HAMILTONIANS

We begin this section by discussing the simulation of

$$e^{-i(H_1+H_2)t},$$

where  $H_1, H_2$  are given Hamiltonians. Restricting the analysis to  $m = 2$  will allow us to illustrate the main idea in our approach while avoiding the rather complicated notation needed in the general case, for  $m \geq 2$ . The simulation of the Schrödinger equation of a  $p$ -particle system, where  $H_1$  is obtained from the Laplacian operator and  $H_2$  is the potential, requires one to consider an evolution operator that has the form above; see [3].

In the next section we deal with the more general simulation problem involving a sum of  $m$  Hamiltonians,  $H_1, \dots, H_m$ , as Berry et al. [4] did, and we will show how to improve their complexity results.

Suzuki proposed methods for decomposing exponential operators in a number of papers [12, 13]. For sufficiently small  $\Delta t$ , starting from the formula

$$S_2(H_1, H_2, \Delta t) = e^{-iH_1\Delta t/2} e^{-iH_2\Delta t} e^{-iH_1\Delta t/2},$$

and proceeding recursively, Suzuki defines

$$S_{2k}(H_1, H_2, \Delta t) = [S_{2k-2}(H_1, H_2, p_k \Delta t)]^2 S_{2k-2}(H_1, H_2, (1 - 4p_k) \Delta t) [S_{2k-2}(H_1, H_2, p_k \Delta t)]^2,$$

for  $k = 2, 3, \dots$ , where  $p_k = (4 - 4^{1/(2k-1)})^{-1}$ , and then proves that

$$\|e^{-i(H_1+H_2)\Delta t} - S_{2k}(H_1, H_2, \Delta t)\| = O(|\Delta t|^{2k+1}). \quad (2)$$

Suzuki was particularly interested in the order of his method, which is  $2k + 1$ , and did not address the size of the implied asymptotic factors in the big- $O$  notation. However, these factors depend on the norms of  $H_1$  and  $H_2$  and can be very large, when  $H_1$  and  $H_2$  do not commute. For instance, when  $H_1$  is obtained from the discretization of the Laplacian operator with mesh size  $h$ ,  $\|H_1\|$  grows as  $h^{-2}$ . Since  $h = \epsilon$ , we get  $\|H_1\| = O(\frac{1}{\epsilon^2})$ . Hence, for fine discretizations  $\|H_1\|$  is huge, and severely affects the error bound above.

Suppose  $\|H_1\| \geq \|H_2\|$ . Since

$$e^{-i(H_1+H_2)t} = e^{-i(\mathcal{H}_1+\mathcal{H}_2)\|H_1\|t},$$

where  $\mathcal{H}_j = H_j/\|H_1\|$ , for  $j = 1, 2$ , we can consider the simulation problem for  $\mathcal{H}_1 + \mathcal{H}_2$  with an evolution time  $\tau = \|H_1\|t$ .

Unwinding the recurrence in Suzuki's construction yields

$$S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t) = \prod_{\ell=1}^K S_2(\mathcal{H}_1, \mathcal{H}_2, z_\ell \Delta t) = \prod_{\ell=1}^K [e^{-i\mathcal{H}_1 z_\ell \Delta t/2} e^{-i\mathcal{H}_2 z_\ell \Delta t} e^{-i\mathcal{H}_1 z_\ell \Delta t/2}], \quad (3)$$

where  $K = 5^{k-1}$  and each  $z_\ell$  is defined according to the recursive scheme,  $\ell = 1, \dots, K$ . In particular,  $z_1 = z_K = \prod_{r=2}^k p_r$ , and for the intermediate values of  $\ell$  the  $z_\ell$  is a product of  $k-1$  factors and has the form  $z_\ell = \prod_{r \in I_0} p_r \prod_{r \in I_1} (1 - 4p_r)$ , where the products are over the index sets  $I_0, I_1$  defined by traversing the corresponding to  $\ell$  path of the recursion tree.

Let  $q_r = \max\{p_r, 4p_r - 1\}$ ,  $r \geq 2$ . Then  $\{q_r\}$  is a decreasing sequence of positive numbers and from [14, p. 18] we have that

$$\frac{3}{3^k} \leq \prod_{r=2}^k q_r \leq \frac{4k}{3^k}.$$

Thus

$$|z_\ell| \leq \frac{4k}{3^k} \quad \text{for all } \ell = 1, \dots, K. \quad (4)$$

Equation (3) can be expressed in the more compact form which we use to simplify the notation. Namely,

$$S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t) = e^{-i\mathcal{H}_1 s_0 \Delta t} e^{-i\mathcal{H}_2 z_1 \Delta t} e^{-i\mathcal{H}_1 s_1 \Delta t} \dots e^{-i\mathcal{H}_2 z_K \Delta t} e^{-i\mathcal{H}_1 s_K \Delta t}, \quad (5)$$

where  $s_0 = z_1/2$ ,  $s_j = (z_j + z_{j+1})/2$ ,  $j = 1, \dots, K-1$ , and  $s_K = z_K/2$ . Observe that  $\sum_{j=0}^K s_j = 1$ ,  $\sum_{j=1}^K z_j = 1$ .

We need to bound  $\sigma_k = \sum_{j=0}^K |s_j| + \sum_{j=1}^K |z_j|$  from above. From (4) we have

$$\sum_{j=1}^K |z_j| \leq \frac{4k5^{k-1}}{3^k},$$

and also

$$\sum_{j=0}^K |s_j| \leq \frac{4k5^{k-1}}{3^k}.$$

Thus

$$\sigma_k \leq \frac{8}{3}k \left(\frac{5}{3}\right)^{k-1} =: c_k \quad \text{for } k \geq 1. \quad (6)$$

(The above trivially holds for  $k = 1$ .)

Expanding each exponential in (5) we obtain

$$\begin{aligned} S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t) = & (I + \mathcal{H}_1 s_0 (-i\Delta t) + \frac{1}{2} \mathcal{H}_1^2 s_0^2 (-i\Delta t)^2 + \dots + \frac{1}{k!} \mathcal{H}_1^k s_0^k (-i\Delta t)^k + \dots) \\ & (I + \mathcal{H}_2 z_1 (-i\Delta t) + \frac{1}{2} \mathcal{H}_2^2 z_1^2 (-i\Delta t)^2 + \dots + \frac{1}{k!} \mathcal{H}_2^k z_1^k (-i\Delta t)^k + \dots) \\ & (I + \mathcal{H}_1 s_1 (-i\Delta t) + \frac{1}{2} \mathcal{H}_1^2 s_1^2 (-i\Delta t)^2 + \dots + \frac{1}{k!} \mathcal{H}_1^k s_1^k (-i\Delta t)^k + \dots) \\ & \dots \\ & (I + \mathcal{H}_2 z_K (-i\Delta t) + \frac{1}{2} \mathcal{H}_2^2 z_K^2 (-i\Delta t)^2 + \dots + \frac{1}{k!} \mathcal{H}_2^k z_K^k (-i\Delta t)^k + \dots) \\ & (I + \mathcal{H}_1 s_K (-i\Delta t) + \frac{1}{2} \mathcal{H}_1^2 s_K^2 (-i\Delta t)^2 + \dots + \frac{1}{k!} \mathcal{H}_1^k s_K^k (-i\Delta t)^k + \dots). \end{aligned} \quad (7)$$

After carrying out the multiplications we see that  $S_{2k}$  is a sum of terms that has the form

$$\frac{s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}}{\alpha_0! \alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!} \mathcal{H}_1^{\alpha_0} \mathcal{H}_2^{\beta_1} \mathcal{H}_1^{\alpha_1} \cdots \mathcal{H}_2^{\beta_K} \mathcal{H}_1^{\alpha_K} (-i\Delta t)^{\sum_{i=0}^K \alpha_i + \sum_{j=1}^K \beta_j}, \quad (8)$$

where the  $\alpha_0, \alpha_1, \dots, \alpha_K$  and the  $\beta_1, \dots, \beta_K$  are obtained by multiplying the denominators in the expansion of the exponentials.

The terms that do not contain  $\mathcal{H}_2$  are those for which  $\beta_1 = \beta_2 = \dots = \beta_K = 0$ , and their sum is

$$\begin{aligned} & \sum_{\alpha_0, \alpha_1, \dots, \alpha_K} \frac{s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K}}{\alpha_0! \alpha_1! \cdots \alpha_K!} \mathcal{H}_1^{\sum_{j=0}^K \alpha_j} (-i\Delta t)^{\sum_{j=0}^K \alpha_j} \\ &= \sum_{\alpha_0} \frac{1}{\alpha_0!} \mathcal{H}_1^{\alpha_0} (-is_0\Delta t)^{\alpha_0} \cdot \sum_{\alpha_1} \frac{1}{\alpha_1!} \mathcal{H}_1^{\alpha_1} (-is_1\Delta t)^{\alpha_1} \cdots \sum_{\alpha_K} \frac{1}{\alpha_K!} \mathcal{H}_1^{\alpha_K} (-is_K\Delta t)^{\alpha_K} \\ &= \prod_{j=0}^K e^{-i\mathcal{H}_1 s_j \Delta t} = \exp(-i \sum_{j=0}^K \mathcal{H}_1 s_j \Delta t) = \exp(-i\mathcal{H}_1 \Delta t). \end{aligned} \quad (9)$$

On the other hand, consider

$$e^{-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t} = I + (-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t) + \cdots + \frac{1}{k!} (-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t)^k + \cdots \quad (10)$$

The terms that do not contain  $\mathcal{H}_2$  sum to

$$\sum_{k=0}^{\infty} \frac{1}{k!} \mathcal{H}_1^k (-i\Delta t)^k = e^{-i\mathcal{H}_1 \Delta t}. \quad (11)$$

Let us now consider the bound in (2). Clearly the terms that do not contain  $\mathcal{H}_2$  cancel out. Therefore, the error is proportional to  $\|\mathcal{H}_2\| |\Delta t|^{2k+1}$ , i.e. it depends on the ratio  $\|\mathcal{H}_2\|/\|\mathcal{H}_1\|$  of the norms of the original Hamiltonians. This fact will be used to improve the error and complexity results of Berry et al. [4]

**Lemma 1.** For  $k \in \mathbb{N}$ ,  $c_k |\Delta t| \leq k + 1$  (see, Eq. 6) and  $\|\mathcal{H}_2\| \leq \|\mathcal{H}_1\| = 1$  we have

$$\|\exp(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t) - S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t)\| \leq \frac{4\|\mathcal{H}_2\|}{(2k+1)!} (c_k |\Delta t|)^{2k+1}. \quad (12)$$

*Proof.* For notational convenience we use  $S_{2k}(\Delta t)$  to denote  $S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t)$ . Consider

$$\exp(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t) - S_{2k}(\Delta t) = \sum_{l=2k+1}^{\infty} [R_l(\Delta t) - T_l(\Delta t)], \quad (13)$$

where  $R_l(\Delta t)$  is the sum of all terms in  $\exp(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t)$  corresponding to  $\Delta t^l$  and  $T_l(\Delta t)$  is the sum of all terms in  $S_{2k}(\Delta t)$  corresponding to  $\Delta t^l$ . Moreover, we know that the terms with only  $\mathcal{H}_1$  cancel out. Hence, we can ignore the terms in  $T_l(\Delta t)$  and  $R_l(\Delta t)$  that contain only  $\mathcal{H}_1$  (and not  $\mathcal{H}_2$ ) as a factor. It follows that

$$R_l(\Delta t) = \frac{1}{l!} (\mathcal{H}_1 + \mathcal{H}_2)^l (-i\Delta t)^l - \frac{1}{l!} \mathcal{H}_1^l (-i\Delta t)^l. \quad (14)$$

Then

$$\|R_l(\Delta t)\| \leq \frac{1}{l!} 2^l \|\mathcal{H}_2\| |\Delta t|^l, \quad (15)$$

since there are  $2^l - 1$  terms, and they are bounded by  $\frac{1}{l!} \|\mathcal{H}_2\| |\Delta t|^l$ .

Now consider the terms in  $T_l(\Delta t)$ . From (7,8)

$$T_l(\Delta t) = \sum_{\sum_{i=0}^K \alpha_i + \sum_{i=1}^K \beta_i = l, \sum_{i=1}^K \beta_i \neq 0} \frac{s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}}{\alpha_0! \alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!} \mathcal{H}_1^{\alpha_0} \mathcal{H}_2^{\beta_1} \mathcal{H}_1^{\alpha_1} \cdots \mathcal{H}_2^{\beta_K} \mathcal{H}_1^{\alpha_K} (-i\Delta t)^l, \quad (16)$$

where the condition  $\sum_{i=1}^K \beta_i \neq 0$  hold because there are no terms containing  $\mathcal{H}_1$  alone. Since the norm of  $\mathcal{H}_1^{\alpha_0} \mathcal{H}_2^{\beta_1} \mathcal{H}_1^{\alpha_1} \cdots \mathcal{H}_2^{\beta_K} \mathcal{H}_1^{\alpha_K}$  is at most  $\|\mathcal{H}_2\|$ , we have

$$\|T_l(\Delta t)\| \leq \sum_{\sum_{i=0}^K \alpha_i + \sum_{i=1}^K \beta_i = l} \frac{|s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}|}{\alpha_0! \alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!} \|\mathcal{H}_2\| |\Delta t|^l. \quad (17)$$

Note that we relaxed the condition  $\sum_{i=1}^K \beta_i \neq 0$  since it does not affect the inequality.

To calculate the sum  $\sum \frac{|s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}|}{\alpha_0! \alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!}$ , where  $\sum_{i=0}^K \alpha_i + \sum_{i=1}^K \beta_i = l$ , we first consider the following equation

$$\begin{aligned} & \exp(|s_0 \Delta t|) \exp(|z_1 \Delta t|) \exp(|s_1 \Delta t|) \cdots \exp(|z_K \Delta t|) \exp(|s_K \Delta t|) \\ &= \left( \sum_{\alpha_0=0}^{\infty} \frac{1}{\alpha_0!} |s_0 \Delta t|^{\alpha_0} \right) \cdot \left( \sum_{\beta_1=0}^{\infty} \frac{1}{\beta_1!} |z_1 \Delta t|^{\beta_1} \right) \cdot \left( \sum_{\alpha_1=0}^{\infty} \frac{1}{\alpha_1!} |s_1 \Delta t|^{\alpha_1} \right) \cdots \\ & \quad \cdots \left( \sum_{\beta_K=0}^{\infty} \frac{1}{\beta_K!} |z_K \Delta t|^{\beta_K} \right) \cdot \left( \sum_{\alpha_K=0}^{\infty} \frac{1}{\alpha_K!} |s_K \Delta t|^{\alpha_K} \right) \\ &= \sum_{p=0}^{\infty} \sum_{\sum \alpha_j + \sum \beta_j = p} \frac{|s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}|}{\alpha_0! \alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!} |\Delta t|^p. \end{aligned} \quad (18)$$

Hence  $\sum_{\sum \alpha_j + \sum \beta_j = l} \frac{|s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}|}{\alpha_0! \alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!}$  is the coefficient of  $|\Delta t|^l$  in the equation above. Similarly,

$$\begin{aligned} & \exp(|s_0 \Delta t|) \exp(|z_1 \Delta t|) \exp(|s_1 \Delta t|) \cdots \exp(|z_K \Delta t|) \exp(|s_K \Delta t|) \\ &= \exp\left(\left(\sum_{i=0}^K |s_i| + \sum_{i=1}^K |z_i|\right) |\Delta t|\right) = \exp(\sigma_k |\Delta t|) \\ &= \sum_{p=0}^{\infty} \frac{1}{p!} \sigma_k^p |\Delta t|^p, \end{aligned} \quad (19)$$

Recall that the bound for  $\sigma_k$  given in Eq. (6). Thus the coefficient of  $|\Delta t|^l$  is bounded from above by  $\frac{1}{l!} c_k^l$ . Therefore, we have

$$\|T_l(\Delta t)\| \leq \frac{c_k^l}{l!} \|\mathcal{H}_2\| |\Delta t|^l. \quad (20)$$

We combine Eq. (15), (20), to obtain

$$\begin{aligned}
\|\exp((\mathcal{H}_1 + \mathcal{H}_2)\Delta t) - S_{2k}(\Delta t)\| &\leq \sum_{l=2k+1}^{\infty} \|R_l(\Delta t) - T_l(\Delta t)\| \\
&\leq \sum_{l=2k+1}^{\infty} \|R_l(\Delta t)\| + \|T_l(\Delta t)\| \\
&\leq 2 \sum_{l=2k+1}^{\infty} \frac{c_k^l}{l!} \|\mathcal{H}_2\| |\Delta t|^l \\
&\leq \frac{2}{(2k+1)!} \|\mathcal{H}_2\| |c_k \Delta t|^{2k+1} \left(1 - \frac{c_k |\Delta t|}{2k+2}\right)^{-1} \\
&\leq \frac{4}{(2k+1)!} \|\mathcal{H}_2\| |c_k \Delta t|^{2k+1},
\end{aligned} \tag{21}$$

where the last two inequalities follow from the assumption  $c_k |\Delta t| \leq k+1$ . and an estimate of the tail of the Poisson distribution; see, e.g., [15, Thm 1].  $\square$

**Theorem 1.** *Let  $1 \geq \varepsilon > 0$  be such that  $8et\|\mathcal{H}_2\| \geq \varepsilon$ . The number  $N$  of exponentials for the simulation of  $e^{-i(H_1+H_2)t}$  with accuracy  $\varepsilon$  is bounded as follows*

$$N \leq 3 \cdot 5^{k-1} \left\lceil \|\mathcal{H}_1\| t \left( \frac{8et\|\mathcal{H}_2\|}{\varepsilon} \right)^{1/(2k)} \frac{8e}{3} \left( \frac{5}{3} \right)^{k-1} \right\rceil,$$

for any  $k \in \mathbb{N}$ , where  $\|\mathcal{H}_2\| \leq \|\mathcal{H}_1\|$ .

*Proof.* Let  $M = |\Delta t|^{-1}$ . Then using Lemma 1 and  $\mathcal{H}_j = H_j/\|\mathcal{H}_1\|$ ,  $j = 1, 2$ , we obtain

$$\begin{aligned}
\|e^{-i(H_1+H_2)t} - S_{2k}^M\| &\leq M \|\mathcal{H}_1\| t \frac{4}{(2k+1)!} \|\mathcal{H}_2\| \left( \frac{c_k}{M} \right)^{2k+1} \\
&= 4t \|\mathcal{H}_2\| \frac{c_k^{2k+1}}{(2k+1)!} \frac{1}{M^{2k}}.
\end{aligned}$$

Recall that  $c_k$  is defined in (6) and is used in Lemma 1. For accuracy  $\varepsilon$  we obtain

$$M \geq \left( \frac{4t \|\mathcal{H}_2\| c_k^{2k+1}}{\varepsilon (2k+1)!} \right)^{1/(2k)}.$$

We use Stirling's formula [16, p. 257] for the factorial function

$$(2k+1)! = \sqrt{2\pi} (2k+1)^{(2k+1)+1/2} e^{-(2k+1)+\theta/(12(2k+1))}, \quad 0 < \theta < 1,$$

which yields

$$[(2k+1)!]^{-1/(2k)} \leq e^{1+1/(2k)}/(2k+1). \tag{22}$$

It is easy to check that

$$c_k^{1/(2k)} \leq 2^{1+1/(2k)}.$$

Thus it suffices to take

$$M \geq \left( \frac{8et\|\mathcal{H}_2\|}{\varepsilon} \right)^{1/(2k)} \frac{2e c_k}{2k+1}.$$

So we define  $M$  to be lower bound of the expression above, i.e.,

$$M := \left( \frac{8et\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{2e c_k}{2k+1}.$$

It is easy to check that

$$\frac{2e}{2k+1}(k+1) \geq e,$$

which along with the condition  $8et\|H_2\| \geq \varepsilon$  yields  $M(k+1) \geq c_k$ . This shows the assumptions of Lemma 1 are satisfied with this value of  $M$ .

From the recurrence relation the number of required exponentials to implement  $S_{2k}$  in one subinterval is no more than  $3 \cdot 5^{k-1}$ . We need to consider two cases concerning  $M\|H_1\|t$ . If  $M\|H_1\|t \geq 1$ , then the number of subintervals is  $\lceil M\|H_1\|t \rceil$ , i.e., we partition the entire time interval into an integer number of subintervals, each of length at most  $M^{-1}$ . The total number of required exponentials is bounded by  $3 \cdot 5^{k-1} \lceil M\|H_1\|t \rceil$ . Substituting the values of  $M$  and  $c_k$  we obtain the bound for  $N$ . In particular,

$$N \leq 3 \cdot 5^{k-1} \left\lceil \|H_1\|t \left( \frac{8et\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{8e}{3} \left( \frac{5}{3} \right)^{k-1} \right\rceil. \quad (23)$$

If  $M\|H_1\|t < 1$ , then Lemma 1 can be used with  $\Delta t = \|H_1\|t$ , since  $\|H_1\|t \leq M^{-1}$  and we have already seen that  $M$  is such that the assumptions of Lemma 1 are satisfied. Thus

$$\begin{aligned} \|e^{-i(H_1+H_2)t} - S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \|H_1\|t)\| &\leq \frac{4}{(2k+1)!} \|\mathcal{H}_2\| (c_k\|H_1\|t)^{2k+1} \\ &= 4t\|H_2\| \frac{c_k^{2k+1}}{(2k+1)!} (\|H_1\|t)^{2k} \leq 4t\|H_2\| \frac{c_k^{2k+1}}{(2k+1)!} (M)^{-2k} \leq \varepsilon, \end{aligned}$$

where the last inequality holds by definition of  $M$ . In this case the total number of exponentials is simply

$$N \leq 3 \cdot 5^{k-1}. \quad (24)$$

Combining (23) and (24) we obtain

$$N \leq 3 \cdot 5^{k-1} \left\lceil \|H_1\|t \left( \frac{8et\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{8e}{3} \left( \frac{5}{3} \right)^{k-1} \right\rceil.$$

This completes the proof.  $\square$

**Remark 1.** Lemma 1 and Theorem 1 indicate that when  $\|H_2\|t \ll \varepsilon$  then the number of exponentials  $N$  can be further improved. In this case it can be shown that high order splitting methods may lose their advantage. We do not pursue this direction in this paper since we assume that the  $H_j$ ,  $j = 1, \dots, m$ , are fixed and study  $N$  as  $\varepsilon \rightarrow 0$ .

### III. SPLITTING METHODS FOR SIMULATING THE SUM OF MANY HAMILTONIANS

In this section we deal with the simulation of

$$e^{-i\sum_{j=1}^m H_j t},$$



where  $H_j$ ,  $j = 1, \dots, m$ , are given non-commuting Hamiltonians. The analysis and the conclusions are similar to those of the previous section where  $m = 2$ , but the proofs are much more complicated and certainly tedious. This is the problem that Berry et al. [4] considered.

We use Suzuki's recursive construction once more [13]. In particular, for

$$S_2(H_1, \dots, H_m, \Delta t) = \prod_{j=1}^m e^{-iH_j \Delta t/2} \prod_{j=m}^1 e^{-iH_j \Delta t/2},$$

and

$$S_{2k}(H_1, \dots, H_m, \Delta t) = [S_{2k-2}(p_k \Delta t)]^2 S_{2k-2}((1 - 4p_k) \Delta t) [S_{2k-2}(p_k \Delta t)]^2, \quad k = 2, 3, \dots,$$

where for notational convenience we have used  $S_{2k-2}(\Delta t)$  to denote  $S_{2k-2}(H_1, \dots, H_m, \Delta t)$ , and  $p_k = (4 - 4^{1/(2k-1)})^{-1}$ , we have that

$$\|e^{-i \sum_{j=1}^m H_j \Delta t} - S_{2k}(H_1, \dots, H_m, \Delta t)\| = O(|\Delta t|^{2k+1}). \quad (25)$$

Assuming again that  $\|H_1\| \geq \|H_2\| \geq \dots \geq \|H_m\|$  we normalize the Hamiltonians by setting  $\mathcal{H}_j = H_j / \|H_1\|$ ,  $j = 1, \dots, m$ , and consider the equivalent simulation problem

$$e^{-i \sum_{j=1}^m \mathcal{H}_j \tau},$$

where  $\tau = \|H_1\|t$ . Proceeding in a way similar to that for  $m = 2$  of the previous section we derive the following lemma, whose proof can be found in the Appendix.

**Lemma 2.** For  $k \in \mathbb{N}$ ,  $d_k |\Delta t| \leq k + 1$ ,  $d_k = m(4/3)k(5/3)^{k-1}$  and  $\|\mathcal{H}_m\| \leq \dots \leq \|\mathcal{H}_2\| \leq \|\mathcal{H}_1\| = 1$  we have

$$\|\exp(-i \sum_{j=1}^m \mathcal{H}_j \Delta t) - S_{2k}(\mathcal{H}_1, \dots, \mathcal{H}_m, \Delta t)\| \leq \frac{4\|\mathcal{H}_2\|}{(2k+1)!} (d_k |\Delta t|)^{2k+1}. \quad (26)$$

From Lemma 2, we have the following theorem.

**Theorem 2.** Let  $1 \geq \varepsilon > 0$  be such that  $4met\|H_2\| \geq \varepsilon$ . The number  $N$  of exponentials for the simulation of  $e^{-i(H_1 + \dots + H_m)t}$  with accuracy  $\varepsilon$  is bounded by

$$N \leq (2m-1) 5^{k-1} \left[ \|H_1\|t \left( \frac{4emt\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{4me}{3} \left( \frac{5}{3} \right)^{k-1} \right],$$

for any  $k \in \mathbb{N}$ , where  $\|H_m\| \leq \dots \leq \|H_2\| \leq \|H_1\|$ .

*Proof.* The proof is similar to that of Theorem 1. Let  $M = |\Delta t|^{-1}$ . Then using Lemma 2 and  $\mathcal{H}_j = H_j / \|H_1\|$ ,  $j = 1, \dots, m$ , we obtain

$$\begin{aligned} \|e^{-i(H_1 + \dots + H_m)t} - S_{2k}^{M\|H_1\|t}(\mathcal{H}_1, \dots, \mathcal{H}_m, 1/M)\| &\leq M\|H_1\|t \frac{4}{(2k+1)!} \|\mathcal{H}_2\| \left( \frac{d_k}{M} \right)^{2k+1} \\ &= 4t\|H_2\| \frac{d_k^{2k+1}}{(2k+1)!} \frac{1}{M^{2k}}. \end{aligned}$$

Recall that  $d_k$  is defined in Lemma 2. For accuracy  $\varepsilon$  we obtain

$$M \geq \left( \frac{4t \|H_2\| d_k^{2k+1}}{\varepsilon (2k+1)!} \right)^{1/(2k)}.$$

We use the estimate (22). It is easy to check that

$$d_k^{1/(2k)} \leq 2m^{1/(2k)}.$$

Thus it suffices to take

$$M \geq \left( \frac{4emt \|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{2e d_k}{2k+1}.$$

So we define  $M$  to be the lower bound of the expression above, i.e.,

$$M := \left( \frac{4emt \|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{2e d_k}{2k+1}.$$

As in the proof of Theorem 1, it is straightforward to verify that  $M(k+1) \geq d_k$ . Therefore, the assumptions of Lemma 2 are satisfied for this value of  $M$ .

From the recurrence relation, we see that the number of required exponentials to implement  $S_{2k}$  in one subinterval is no more than  $(2m-1) \cdot 5^{k-1}$ . Again we distinguish two cases for  $M \|H_1\| t$ . We deal with the case  $M \|H_1\| t < 1$  in the same way we did in the proof of Theorem 1, to conclude

$$N \leq (2m-1) \cdot 5^{k-1}.$$

If  $M \|H_1\| t \geq 1$ , then the total number of required exponentials is

$$N \leq (2m-1) \cdot 5^{k-1} \lceil M \|H_1\| t \rceil.$$

Substituting the values of  $M$  and  $d_k$  we obtain

$$N \leq (2m-1) \cdot 5^{k-1} \left\lceil \|H_1\| t \left( \frac{4emt \|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{4me}{3} \left( \frac{5}{3} \right)^{k-1} \right\rceil.$$

This completes the proof.  $\square$

The reader may wish to recall Remark 1 that applies in the case too.

**Corollary 1.** *If in addition to the assumptions of Theorem 2 either of the following two conditions holds:*

- $4met \|H_1\| \geq 3$
- $\varepsilon$  is sufficiently small such that

$$\left( \ln \frac{4met \|H_1\|}{5} \right)^2 - 2 \ln \frac{5}{3} \ln \frac{4met \|H_2\|}{\varepsilon} < 0$$

*then the number of exponentials,  $N$ , for the simulation of  $e^{-i(H_1+\dots+H_m)t}$  with accuracy  $\varepsilon$  is bounded by*

$$N \leq 2 (2m-1) 5^{k-1} \|H_1\| t \left( \frac{4emt \|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{4me}{3} \left( \frac{5}{3} \right)^{k-1},$$

*for any  $k \in \mathbb{N}$ .*

*Proof.* From the assumption of Theorem 2 we have  $4emt\|H_2\|/\varepsilon \geq 1$ . Consider the argument of the ceiling function in the bound of Theorem 2. It is greater than or equal to 1, if  $4met\|H_1\| \geq 3$ . Otherwise, we take its logarithm and multiply the resulting expression by  $k$ . This gives the quadratic polynomial

$$2k^2 \ln \frac{5}{3} + 2k \ln \frac{4met\|H_1\|}{5} + \ln \frac{4met\|H_2\|}{\varepsilon}.$$

When  $\varepsilon$  is sufficiently small and the discriminant is negative, i.e., when

$$\left( \ln \frac{4met\|H_1\|}{5} \right)^2 - 2 \ln \frac{5}{3} \ln \frac{4met\|H_2\|}{\varepsilon} < 0,$$

the polynomial is positive for all  $k$ . Hence, that argument of the ceiling function in the bound of Theorem 2 is greater than 1, for all  $k \geq 1$ .

In either case, we use  $\lceil x \rceil \leq 2x$ , for  $x \geq 1$ , to estimate  $N$  from above.  $\square$

#### IV. SPEEDUP

Let us now deal with the cost for simulating the evolution  $e^{-i(\sum_{j=1}^m H_j)t}$ . Berry et al. [4] show upper and lower bounds for the number of required exponentials. We concentrate on upper bounds and improve the estimates of [4].

We are interested in the number of exponentials required by the splitting formula that approximates the evolution with accuracy  $\varepsilon$ . Recall that

$$N_{\text{new}} := 2(2m-1)5^{k-1}\|H_1\|t \left( \frac{4emt\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{4me}{3} \left( \frac{5}{3} \right)^{k-1}$$

exponentials suffice for error  $\varepsilon$ . The above estimate holds for  $\varepsilon$  sufficiently small as Theorem 2 and Corollary 1 indicate. The corresponding previously known estimate [4] is

$$N_{\text{prev}} = m 5^{2k} (m\|H_1\|t)^{1+\frac{1}{2k}} \left( \frac{1}{\varepsilon} \right)^{\frac{1}{2k}},$$

where  $H = \sum_{j=1}^l H_j$ .

The ratio of the two estimates is

$$\frac{N_{\text{new}}}{N_{\text{prev}}} \leq \frac{2}{3^k} \left( \frac{4e\|H_2\|}{\|H_1\|} \right)^{1/2k}. \quad (27)$$

So for large  $k$  we have an improvement in the estimate of the cost of the algorithm. On the other hand, if  $\|H_2\| \ll \|H_1\|$  we have an improvement in the estimate of the cost the algorithm not just for large  $k$  but for all  $k$ . This is particularly significant when  $k$  is small. For instance,  $k = 1$  for the Strang splitting  $S_2$ , which is frequently used in the literature.

Let us now consider the optimal  $k$ , i.e., the one minimizing  $N_{\text{new}}$ , for a given accuracy  $\varepsilon$ . It is obtained from the solution of the equation

$$2k^2 \ln \frac{25}{3} - \ln \frac{4emt\|H_2\|}{\varepsilon} = 0.$$

Since we seek a positive integer  $k_{\text{new}}^*$  minimizing  $N_{\text{new}}$ , we set

$$k_{\text{new}}^* := \max \left\{ \text{round} \left( \sqrt{\frac{1}{2} \log_{25/3} \frac{4emt \|H_2\|}{\varepsilon}} \right), 1 \right\},$$

where  $\text{round}(x) = \lfloor x + 1/2 \rfloor$ ,  $x \geq 0$ . We can avoid using the max function in the expression above by considering  $\varepsilon \leq mt \|H_2\|$ . Then the number of exponentials  $N_{\text{new}}$  satisfies

$$N_{\text{new}}^* \leq \frac{8}{3} (2m - 1) met \|H_1\| e^{2\sqrt{\frac{1}{2} \ln \frac{25}{3} \ln \frac{4emt \|H_2\|}{\varepsilon}}}.$$

Berry et al. [4] find

$$k_{\text{prev}}^* = \text{round} \left( \frac{1}{2} \sqrt{\log_5 \frac{m \|H_1\| t}{\varepsilon} + 1} \right), \quad (28)$$

which minimizes  $N_{\text{pre}}$ . For  $k_{\text{prev}}^*$  the number of exponentials  $N_{\text{prev}}$  becomes

$$N_{\text{prev}}^* = 2m^2 \|H_1\| t e^{2\sqrt{\ln 5 \ln \frac{m \|H_1\| t}{\varepsilon}}}. \quad (29)$$

As a final comparison with  $N_{\text{prev}}$  we have

$$\frac{N_{\text{new}}^*}{N_{\text{prev}}^*} \leq \frac{8e}{3} e^{2\left(\sqrt{\frac{1}{2} \ln \frac{25}{3} \ln \frac{4emt \|H_2\|}{\varepsilon}} - \sqrt{\ln 5 \ln \frac{m \|H_1\| t}{\varepsilon}}\right)}.$$

Hence, there is an important difference between the previously derived optimal  $k$  and the one derived in the present paper. In [4], the optimal  $k$  depends on  $\|H_1\|$ . More precisely, we show that the optimal  $k$  depends on  $\|H_2\|$ , the second largest norm of the Hamiltonians comprising  $H$ , which can be considerably smaller than  $\|H_1\|$ .

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## VI. APPENDIX

*Proof of Lemma 2.* Unwinding the recurrence for  $S_{2k}$  we see that

$$S_{2k}(\mathcal{H}_1, \dots, \mathcal{H}_m, \Delta t) = \prod_{\ell=1}^K S_2((\mathcal{H}_1, \dots, \mathcal{H}_m, z_\ell \Delta t)) = \prod_{\ell=1}^K \left[ \prod_{j=1}^m e^{-i\mathcal{H}_j z_\ell \Delta t/2} \prod_{j=m}^1 e^{-i\mathcal{H}_j z_\ell \Delta t/2} \right],$$

where  $K = 5^{k-1}$  and each  $z_\ell$  is defined according to the recursive scheme,  $\ell = 1, \dots, K$ . For the details, see the part of the text that follows (3). The bound (4), namely,

$$|z_\ell| \leq \frac{4k}{3^k} \quad \text{for all } \ell = 1, \dots, K,$$

holds independently of  $m$ , because it depends on the  $k - 1$ st levels of the recursion tree and not on the leaf,  $S_2((\mathcal{H}_1, \dots, \mathcal{H}_m, z_\ell \Delta t)$ , at which, the corresponding to  $\ell$ , path ends.

In the expression of  $S_2((\mathcal{H}_1, \dots, \mathcal{H}_m, z_\ell \Delta t)$  the sum of the magnitudes of the factors multiplying the Hamiltonians in the exponents is  $m|z_\ell| \cdot |\Delta t|$ , for all  $\ell = 1, \dots, K$ . Thus in the expression of  $S_{2k}$  above, the sum of the magnitudes of all factors multiplying the Hamiltonians in the exponents is

$$\sum_{\ell=1}^K (m|z_\ell| \cdot |\Delta t|) \leq 5^{k-1} m \frac{4k}{3^k} |\Delta t|.$$

Define

$$d_k := m \frac{4}{3} k \left( \frac{5}{3} \right)^{k-1} \quad k \geq 1. \quad (30)$$

Equivalently, one can view the expression for  $S_{2k}$  above as a product of exponentials of the form  $e^{\mathcal{H}_j r_{j,n} \Delta t}$ , where  $\sum_{n=1}^{N_j} r_{j,n} = 1$ ,  $j = 1, \dots, m$ , and  $N_j$  is the number of occurrences of  $\mathcal{H}_j$  in  $S_{2k}$ . Recall that for  $m = 2$  we used  $s_n$  to denote  $r_{1,n}$  and  $z_n$  to denote  $r_{2,n}$ . With this notation and using (30) we have

$$\sum_{j,n} |r_{j,n}| \leq d_k. \quad (31)$$

(Recall the derivation of (6).)

Expanding the factors of  $S_{2k}$  in a power series individually, and then carrying out the multiplications amongst them, we conclude that  $S_{2k}$  is given by an infinite sum whose terms have the form

$$\prod_{(j,n)} \frac{1}{\gamma_{j,n}!} \mathcal{H}_j^{\gamma_{j,n}} [-i r_{j,n} \Delta t]^{\gamma_{j,n}}. \quad (32)$$

The factors of these products are specified by the Hamiltonians  $H_j$  and the order of their occurrences after unwinding the recurrence for  $S_{2k}$ , where  $j = 1, \dots, m$  and  $\gamma_{j,n} = 0, 1, 2, \dots$ , for all  $n = 1, \dots, N_j$ .

Consider the terms that contain only  $\mathcal{H}_1$  and, therefore, have  $\gamma_{j,n} = 0$ , for  $n = 1, \dots, N_j$  and  $j = 2, \dots, m$ . The sum of these terms is

$$\begin{aligned} \sum_{\gamma_{j,n}=0 \text{ for } j \neq 1} \prod_{(j,n)} \frac{1}{\gamma_{j,n}!} \mathcal{H}_j^{\gamma_{j,n}} [-i r_{j,n} \Delta t]^{\gamma_{j,n}} &= \sum_{\gamma_{1,1}=\dots=\gamma_{1,N_1}=0}^{\infty} \prod_{(1,n)} \frac{1}{\gamma_{1,n}!} \mathcal{H}_1^{\gamma_{1,n}} [-i r_{1,n} \Delta t]^{\gamma_{1,n}} \\ &= \prod_{n=1}^{N_1} \sum_{\gamma_{1,n}} \frac{1}{\gamma_{1,n}!} H_1^{\gamma_{1,n}} [-i r_{1,n} \Delta t]^{\gamma_{1,n}} = \prod_{n=1}^{N_1} e^{-i \mathcal{H}_1 r_{1,n} \Delta t} \\ &= e^{-i \sum_n r_{1,n} H_1 \Delta t} = e^{-i \mathcal{H}_1 \Delta t}. \end{aligned} \quad (33)$$

On the other hand,

$$e^{-i \sum_{j=1}^m \mathcal{H}_j \Delta t} = I + \left( -i \sum_{j=1}^m \mathcal{H}_j \Delta t \right) + \dots + \frac{1}{k!} \left( -i \sum_{j=1}^m \mathcal{H}_j \Delta t \right)^k + \dots, \quad (34)$$

and the terms that contain only  $\mathcal{H}_1$  have sum

$$\sum_{k=0}^{\infty} \frac{1}{k!} \mathcal{H}_1^k (-i\Delta t)^k = e^{-i\mathcal{H}_1 \Delta t}. \quad (35)$$

Let us now consider the error bound in (25). The sum of the terms with only  $\mathcal{H}_1$  in  $S_{2k+1}$  and  $\exp(\sum_{j=1}^m H_j \Delta t)$  is the same and cancels out when we subtract one from the other. Moreover, in  $\exp(-i \sum_{j=1}^m \mathcal{H}_j \Delta t) - S_{2k}(\Delta t)$  we know that the terms of order up to  $2k$  also cancel out, see Eq. (25). From this we conclude that the error is proportional to  $\|\mathcal{H}_2\| |\Delta t|^{2k+1}$ .

Consider

$$\exp(-i(\mathcal{H}_1 + \dots + \mathcal{H}_m)\Delta t) - S_{2k}(\mathcal{H}_1, \dots, \mathcal{H}_m, \Delta t) = \sum_{l=2k+1}^{\infty} [R_l(\Delta t) - T_l(\Delta t)], \quad (36)$$

where  $R_l(\Delta t)$  is the sum of all terms in  $\exp(-i(\mathcal{H}_1 + \dots + \mathcal{H}_m)\Delta t)$  corresponding to  $\Delta t^l$  and  $T_l(\Delta t)$  is the sum of all terms in  $S_{2k}$  corresponding to  $\Delta t^l$ . We can ignore the terms in  $T_l(\Delta t)$  and  $R_l(\Delta t)$  that contain only  $\mathcal{H}_1$  (and not  $\mathcal{H}_2$ ) as a factor.

Then

$$\|R_l(\Delta t)\| = \left\| \frac{1}{l!} \left( \sum_{j=1}^m \mathcal{H}_j \Delta t \right)^l - \frac{1}{l!} \mathcal{H}_1^l \Delta t^l \right\| \leq \frac{m^l}{l!} \|\mathcal{H}_2\| |\Delta t|^l, \quad (37)$$

because there are  $m^l - 1$  terms in  $R_l$  and each norm is at most  $\frac{1}{l!} \|\mathcal{H}_2\| |\Delta t|^l$ .

From (32) we have

$$T_l(\Delta t) = \sum_{\sum \gamma_{j,n}=l} \frac{\prod_{(j,n)} r_{j,n}^{\gamma_{j,n}}}{\prod_{(j,n)} \gamma_{j,n}!} \prod_{(j,n)} \mathcal{H}_j^{\gamma_{j,n}} \Delta t^l, \quad (38)$$

where  $\sum_n \gamma_{1,n} \neq l$ , i.e., there is no terms containing only  $\mathcal{H}_1$ . So,  $\|\prod_{(j,n)} \mathcal{H}_j^{\gamma_{j,n}}\| \leq \|\mathcal{H}_2\|$ , and

$$\|T_l(\Delta t)\| \leq \sum_{\sum \gamma_{j,n}=l} \frac{\prod_{j,n} |r_{j,n}|^{\gamma_{j,n}}}{\prod_{j,n} \gamma_{j,n}!} \|\mathcal{H}_2\| |\Delta t|^l. \quad (39)$$

To calculate the coefficients of the sum, we consider

$$\begin{aligned} \prod_{(j,n)} \exp(|r_{j,n} \Delta t|) &= \prod_{(j,n)} \sum_{\gamma_{j,n}=0}^{\infty} \frac{1}{\gamma_{j,n}!} |r_{j,n} \Delta t|^{\gamma_{j,n}} \\ &= \sum_{l=0}^{\infty} \sum_{\sum \gamma_{j,n}=l} \frac{\prod_{j,n} |r_{j,n}|^{\gamma_{j,n}}}{\prod_{j,n} \gamma_{j,n}!} |\Delta t|^l. \end{aligned} \quad (40)$$

Hence the coefficient of  $|\Delta t|^l$  in (39) is equal to that in (40). Also

$$\prod_{j,n} \exp(|r_{j,n} \Delta t|) = \exp\left(\sum_{j,n} |r_{j,n} \Delta t|\right). \quad (41)$$

From (31) we obtain

$$\|T_l(\Delta t)\| = \frac{d_k^l}{l!} \|\mathcal{H}_2\| |\Delta t|^l. \quad (42)$$

Therefore,

$$\begin{aligned}
\|\exp(\sum_{j=1}^m \mathcal{H}_j \Delta t) - S_{2k}(\Delta t)\| &\leq \sum_{l=2k+1}^{\infty} \|R_l(\Delta t)\| + \|T_l(\Delta t)\| \\
&\leq 2 \sum_{l=2k+1}^{\infty} \frac{d_k^l}{l!} \|\mathcal{H}_2\| |\Delta t|^l \\
&= 2 \|\mathcal{H}_2\| \sum_{l=2k+1}^{\infty} \frac{1}{l!} |d_k \Delta t|^l \\
&\leq \frac{2}{(2k+1)!} \|\mathcal{H}_2\| |d_k \Delta t|^{2k+1} \left(1 - \frac{d_k |\Delta t|}{2k+2}\right)^{-1} \\
&\leq \frac{4}{(2k+1)!} \|\mathcal{H}_2\| |d_k \Delta t|^{2k+1},
\end{aligned} \tag{43}$$

where the last two inequalities follow from the assumption  $d_k |\Delta t| \leq k+1$  and an estimate of the tail of the Poisson distribution; see, e.g., [15, Thm 1].  $\square$

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